

RANGE AND STOPPING POWER CALCULATIONS IN NUCLEONICA

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ABSTRACT

In the interaction between charged particles and matter, the stopping power or the average energy loss per unit path length plays an important role in many fields. Because of the great interest in this phenomenon, a web-based application has been developed in the Nucleonica portal to calculate the range and stopping power of electrons, positrons, protons, alphas, muons and heavy ions in a variety of different targets. The target materials can be selected from a variety of pre-defined elements and compounds. Alternatively, user-defined compounds can be created and stored for later use. The present paper provides a detailed description the range and stopping power calculations in Nucleonica. Agreement between the results and other well-known computer codes and experimental results shows that the module gives very reliable results. The application is suitable for professional use and for education and training purposes by educators and students in nuclear science.

1. Introduction

Stopping power, i.e. energy loss of energetic particles per unit length in matter, has been studied experimentally and theoretically since the beginning of the 20th century because of its wide application area, such as ion implantation, fundamental particle physics, nuclear physics, radiation damage, radiology, structure analysis of solid target by Rutherford backscattering spectroscopy, and plasma-first wall interaction in a nuclear-fusion reactor. Stopping power can be considered in two parts: first is the interaction of incident particle with target electrons (called electronic stopping power), and second is the interaction with target nuclei (called nuclear stopping power).

The first (classical) calculation of the energy loss of energetic particles was made by Bohr [1], while the first quantum mechanical treatment was done by Bethe [2]. This latter theory of stopping power is particularly accurate when the projectile's velocity is sufficiently high. Another important quantity is the range of the charged particle in matter. The range is defined as the mean path length of the particle in the target matter before coming to rest. Generally, analytic transport theory and Monte Carlo calculations are used for the range calculations.

Because of its importance, we have developed a web-based application for Range and Stopping Power (R&SP) calculations. One can easily calculate Range and Stopping Power for many types of projectile in various targets through the user-friendly interface in NUCLEONICA [3]. Full documentation of this module is given in the Nucleonica Wiki [4].

2. Projectile-Target Compositions

The user interface of the R&SP module is shown in Fig. 1. All pre-defined parts of module can be selected through the appropriate combo boxes in the main menu. Electrons, positrons, alphas, protons, muons, and ions with atom numbers from 1 to 92 can be selected from the "projectile" combo box shown in Fig. 1.

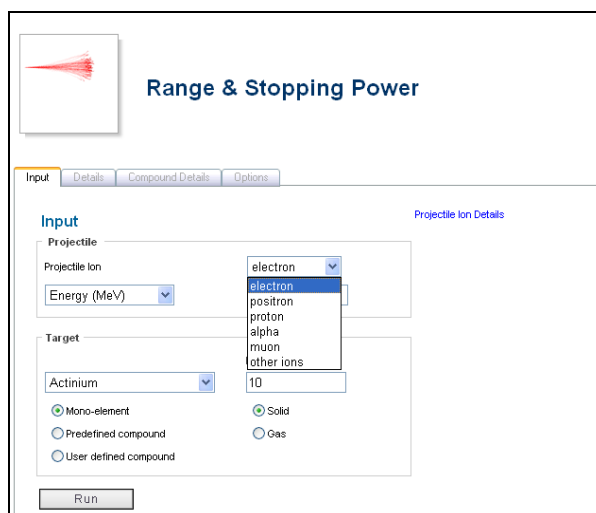
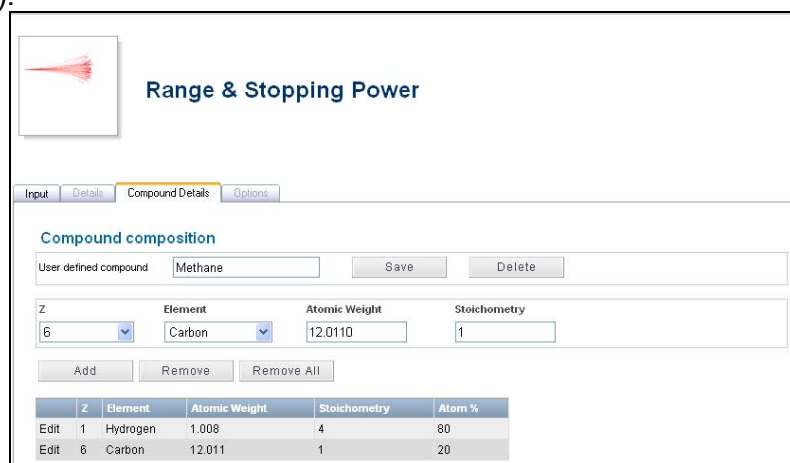


Fig 1. The RANGE module interface showing the types of projectiles available.

If the user selects "other ions", two new combo boxes appear. The first allows the user to choose an element from $Z=1$ to 92 and second allows selection of the isotopes. There are some limitations with regard to setting the energy of projectile. The module does not calculate stopping power and range if the projectile's energy is less than 10 keV or more than 1 GeV for electrons and positrons, and less than 1 MeV or more than 1 GeV for muons, and less than 1 keV or more than 2 GeV for alphas, protons and other ions.

For targets, the user can choose predefined mono-element from $Z=1$ to 92, predefined compounds, or user defined compounds. Pre-defined mono elements and compounds can be selected by using the corresponding radio buttons and combo box. Moreover, the target densities are taken from the Nucleonica database. By selecting the corresponding radio button, gas or solid state atomic density of the target is taken from the database. These values can, however, be changed in the density TextBox in main menu.

Users can create their own compounds by clicking the appropriate radio button and then "Compound Details" menu. In the compound details menu, one can add elements and their corresponding stoichiometry. User defined compounds can be given a name and saved for later use (Fig.2).



	Z	Element	Atomic Weight	Stoichiometry	Atom %
Edit	1	Hydrogen	1.008	4	80
Edit	6	Carbon	12.011	1	20

Fig 2. Interface for the creation of user-defined compounds.

Once the projectile and target have been selected/created, the calculations can be initiated by clicking the "Run" button. The results are then shown at the bottom of the page (see Fig.3).

Fig 3. Main page of the Range module showing the input and summary results.

In addition to the summary results shown in Fig. 3 for a particular energy, the Range module creates a table of results for a wide energy range. This Table (button is shown at the bottom of Fig.3) contains projectile energy, electronic and nuclear stopping powers, the range, and the longitudinal and lateral straggling. Additional information is given in the results "Details" shown in Fig. 3. User can also see the graph of stopping power (Graph SP) and range (Graph Range) for the calculation. More details of the Range module can be found in Nucleonica Wiki [4].

3. Calculation Method and Theories Behind Range Module

The Range module uses different calculation methods depending on the type of the projectile. Mainly the SRIM [5] "engine" is used for heavy ions as well as alphas and protons. SRIM is a well known computer program developed by J.F. Ziegler and Biersack for the calculation of stopping power and range. This program includes many different methods including fitting to the experimental results. A detailed description of the calculation method can be found in *The Stopping and Ranges of Ions in Solids* [6].

In addition, we have used our codes for the calculations for electron, positron and muon projectiles. These calculations depend on previously developed and published methods. For electrons and positrons our codes are based on the work of H. Gümüş et al. [7,8]. Because the positron has the same mass and a charge opposite that of the electron, the structure of a positron track in matter is frequently assumed to be similar to that of an electron, so stopping power is calculated in a similar way to that of the electron. The Stopping Power calculation for electrons (or positrons) which are traversing through matter is similar to that of heavy charged particles. The interaction of incident particles with target electrons can be calculated from Bethe's theory, and this gives rise to the "Collisional Stopping Power". The interaction between incident particles (electrons or positrons) and target nucleus results in Bremsstrahlung, and this gives rise to the "Radiative Stopping Power". The collisional stopping power of matter is calculated by considering the effective charge approximation. When charged particles are accelerated or decelerated, they radiate and the energy of this

radiation can be any value from 0 to the energy of incident particles. This is the source of the radiative stopping power or Bremsstrahlung. This is more important especially for fast electrons (or positrons), since the mass of electron is much lower than that of nucleus it is accelerated more rapidly when it is in the coulomb field of nucleus. The strength of Bremsstrahlung depends on the target's atomic number (Z), and it is proportional to Z^2 and also proportional to incident energies. On the other hand, the collisional stopping power is proportional to Z . So, the ratio of the radiative stopping power to the collisional stopping power is approximately given by

$$\frac{S_{rad}}{S_{coll}} = \frac{ZE}{800} \quad (1)$$

at high energies (more than 10 MeV), and E is the energy of the incident electrons in units of MeV. At high energies, this ratio can be used to calculate the radiative stopping power. The RANGE module uses this ratio to calculate radiative stopping power.

The muon is an elementary particle whose charge ($-1 e$) and spin ($1/2$) are equal to that of the electron. It is sometimes regarded as a "heavy" electron, because its mass is 207 times the electron mass and its interactions with matter are very similar to those of electrons. Muon interactions with matter differ significantly from electron interactions purely as a result of its much greater mass. For example the stopping power for electrons, particularly in the high energy regime, is dominated by the bremsstrahlung process, which is not the case for muons unless the energies are in the multi-GeV range. On the other hand, in this multi-GeV regime, radiative processes are more pronounced than for other heavy charged particles and ions. The Range module uses Bethe-Bloch equation for muons [9] for the calculation of stopping power.

Most of the transport calculations and Monte Carlo simulations for the calculation of Range are based on the so-called **C**ontinuous **S**lowing **D**own **A**pproximation (CSDA). In this approximation, it is assumed that the particle loses its energy in a continuous way and at a rate equal to the stopping power. Since the stopping power is the energy loss of projectile per unit path, CSDA range (or Bethe range) is calculated by

$$R(E) = \int_{E_{abs}}^E \frac{dE'}{S(E')}$$

where E_{abs} is the energy where particle is effectively absorbed. The CSDA range is the path length travelled by the particle and since energy-loss fluctuations are not considered, the CSDA range is always higher than projected range (R_p) which is the distance between the point where particle enters the stopping medium and the point where particle is absorbed (or comes to rest). It becomes important when the projectile's energy is low enough. For electrons, positrons and muons, the Range module uses this approximation to calculate the range of the projectile in the matter.

4. Accuracy of the Range Module

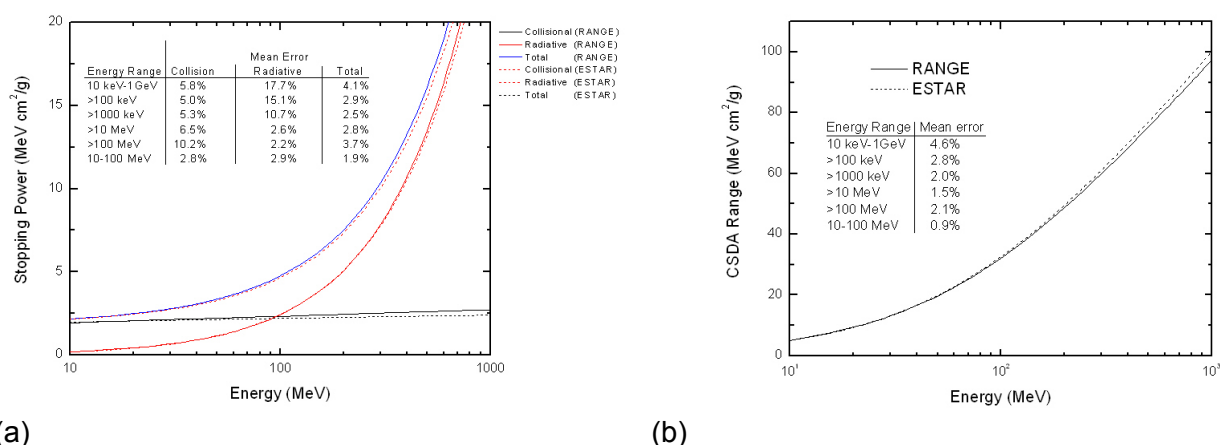
To determine the accuracy of the Range module results, we have compared our results with various results in the literature. For electrons, protons and alphas in gas, solid and liquid phases for mono element and compound targets, we compared our results with the results obtained from the STAR program groups [10]. STAR program groups include three different stopping power and range calculation programs: ESTAR for electrons, PSTAR for protons and ASTAR for alphas. These programs were developed at the NIST. For positrons, we compared our results with the results given in ICRU 37 report [11]. For muons, we compared our results with the results given in Ref. [9]. The Range module uses SRIM for heavy particles with a known accuracy of less than 5%.

Test results show that agreements are less than 5% for protons and alphas, less than 10% for electrons and positrons, and less than 7% for muons. These results show the mean error and are for the total stopping powers and the CSDA Ranges.

For electrons and positrons, agreement is better than these results for collisional stopping power, however, for radiative stopping power mean error is higher because we use the simple ratio (Equation 1) to calculate the radiative stopping power.

For muons, the Range module uses the formulation which is indicated at the work of Groom et al. [9]. Because we calculate the stopping power at the energies below 1 GeV, we have calculated only collisional stopping power. However, the radiative stopping becomes important at high energies, so one must calculate also radiative stopping power. On the other hand, radiative stopping power is important above 100 GeV in almost all matter. This shows that our calculation can be also used at the energies above 1 GeV for muons.

Below, we give the graphs of the results of Range module for electrons in water as an example. The graphs include mean errors in Range module. Results for other projectiles and targets are given in the Nucleonica wiki [4].



(a)

(b)

Fig 4. Range module results for electrons in water (liquid):
(a) the stopping power of water (liquid) (b) the range of electrons

5. Conclusions

The Range module in Nucleonica provides a user-friendly interface for quick and accurate calculations on the range and stopping powers of charged particles - electrons, positrons, protons, alphas, muons and heavy ions - in matter. Target materials include the natural elements, pre-defined and user-defined compounds. In addition, the user can also select the energy and stopping power units, etc. Range and stopping power results can be displayed in high quality graphs. The Range module can be used in the Nucleonica scripting language [12]. A detailed description of the Range module and the underlying theory is given in online Help in the NucleonicaWiki.

6. References

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